FAQs About Hybrid Atomic Orbitals

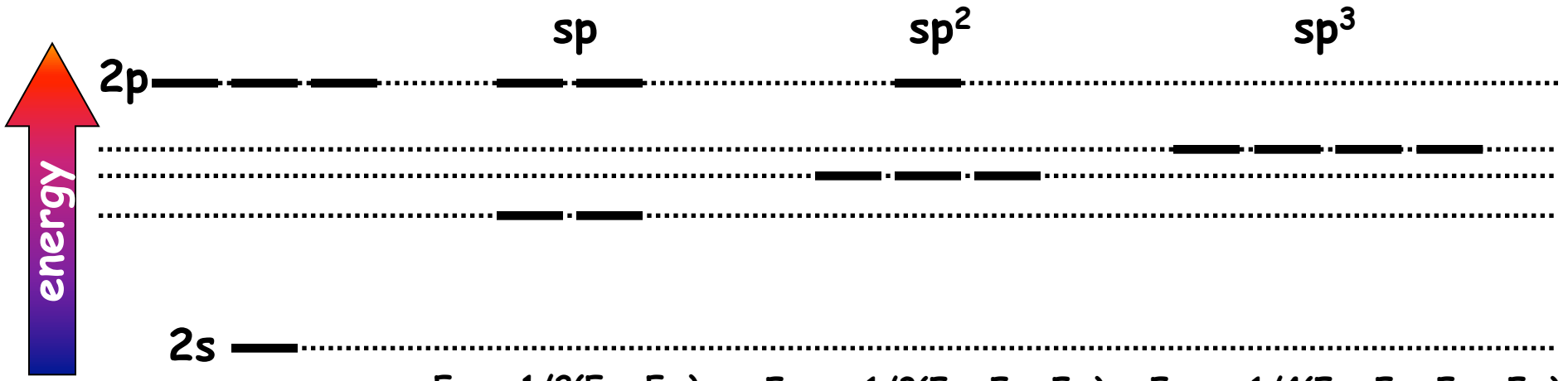
(1) When do I use hydrid orbitals rather than 2s, p_x, p_y, p_z?

Hybrid orbitals are convenient for ideal bonding geometries of complex molecules.

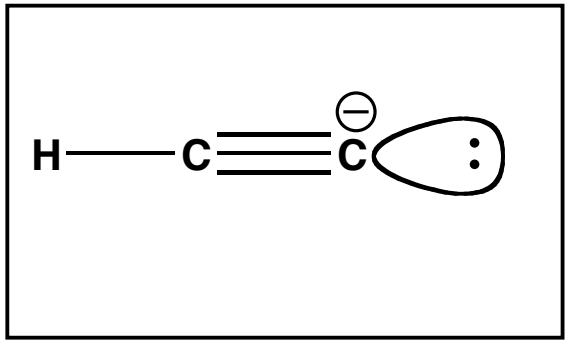
⇒Use 2s, p_x, p_y, p_z for diatomic molecules

⇒Use hybrid orbitals for more complex organic molecules

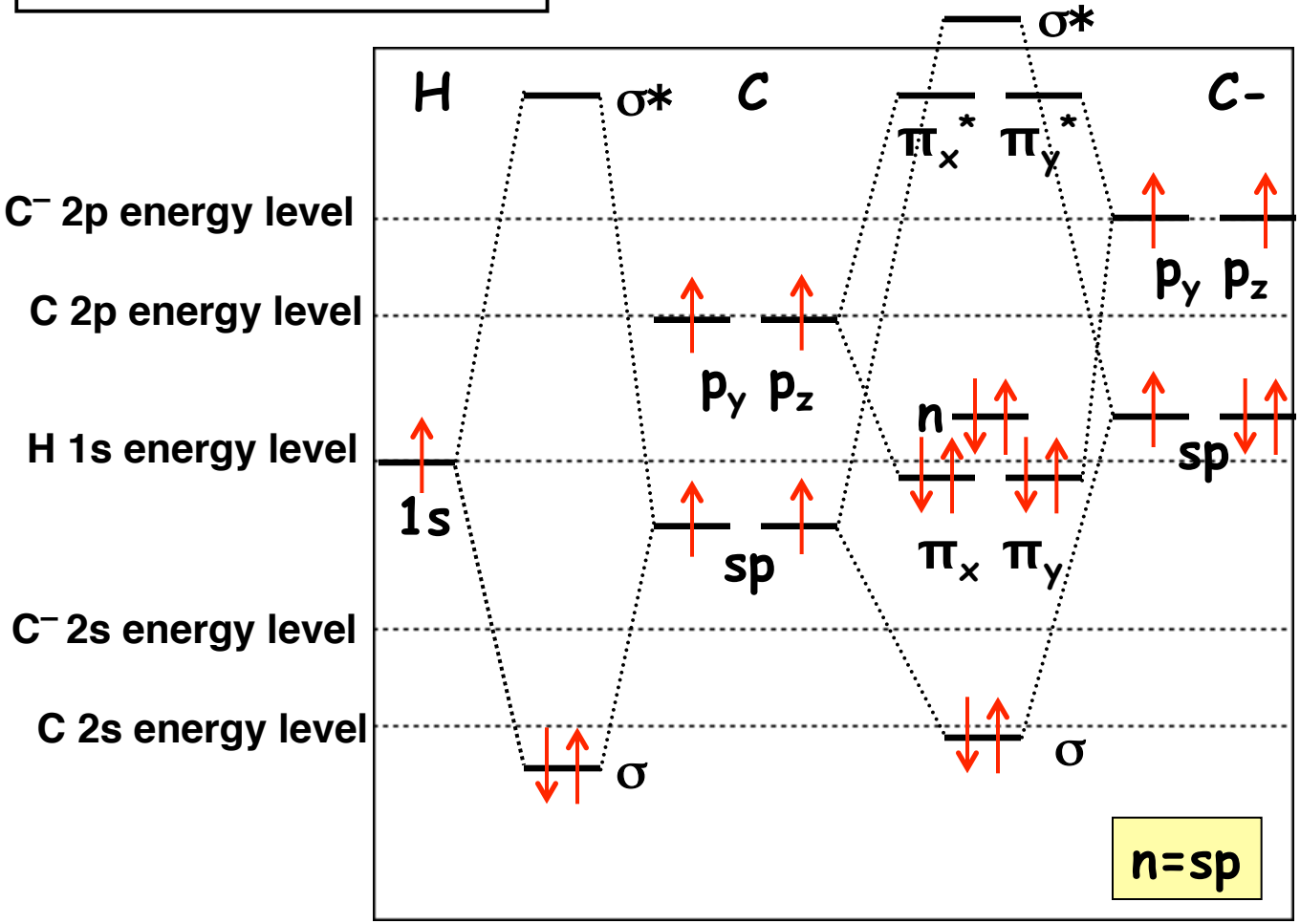
(2) How do I calculate the energy of a hybrid orbital?



MOs from Hybrid AOs



Construct a MO energy diagram for acetylide anion



Guidelines

1) Look up the energy of the AOs; relative to neutral atom, positive charge lowers, energy, negative charge raises energy

2) decide which hybrid AOs to use for each atom (e.g., based on VSEPR geometry)

3) section diagram into regions based on bonds

4) position the hybrid AOs on the energy diagram

- sp 1/2 between 2s and 2p
- sp^2 2/3 between 2s and 2p
- sp^3 3/4 between 2s and 2p

5) use hybrid orbital combinations to construct MOs

- σ / σ* have stronger interactions than π / π* (better overlap in sigma case)
- energy of non-bonded orbital remains unchanged from corresponding AO

6) add electrons following Aufbau method